Solid on Solid Model for Surface Growth in 2+1Dimensions

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Abstract. We analyze in detail the Solid-On-Solid model (SOS) for growth processes on a square substrate in 2+1 dimensions. By using the Markovian surface properties, we introduce an alternative approach for determining the roughness exponent of a special type of SOS model-the Restricted-Solid-On-Solid model (RSOS)- in 2 + 1 dimensions. This model is the SOS model with the additional restriction that the height difference must be S=1. Our numerical results show that the behaviour of the SOS model in 2+1 dimensions for approximately $S \geq S_{\times} \sim 8$ belongs to the two different universality classes: during the initial time stage, $t < t_{\times}$ it belongs to the Random-Deposition (RD) class, while for $t_{\times} < t \ll t_{sat}$ it belongs to the Kardar-Parisi-Zhang (KPZ) universality class. The crossover time (t_{\times}) is related to S via a power law with exponent, $\eta = 1.99 \pm 0.02$ at 1σ confidence level which is the same as that for 1+1 dimensions reported in Ref. [8]. Using the structure function, we compute the roughness exponent. In contrast to the growth exponent, the roughness exponent does not show crossover for different values of S. The scaling exponents of the structure function for fixed values of separation distance versus S in one and two space dimensions are $\xi = 0.92 \pm 0.05$ and $\xi = 0.86 \pm 0.05$ at 1σ confidence level, respectively.

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1. Introduction

Surface growth processes, especially the formation of thin film deposits, have been studied using various approaches in complex systems and statistical analysis [1, 2, 3, 4, 5, 6, 7]. The factors which control surface growth phenomena have immense phase space. Consequently, to be able to analyze these phenomena one needs to make many assumptions, which can lead to results that are unreliable. Combining insights from computational simulation and simplified analysis will likely give better results. It is well-known that the understanding of phenomena such as advances of bacterial colonies, electrochemical deposition, flameless fire fronts and molecular-beam-epitaxial growth is of considerable importance in the control of many interesting growth processes in industries [7, 8, 9]. The simplest surface growth model is the so called statistical deposition model [7, 10]. Some models proposed to explore growth surfaces, such as the Family model [11], Ballistic Deposition(BD) model [12, 13] and the Eden model [14], are able to account for many of the properties of some real systems. For example, the BD and Eden models can accurately simulate vapor deposition and biological growth. However, these models tend to ignore the microscopic details of the interfaces, and cannot provide accurate scaling exponents. In addition many fractal features of real systems remain unexplained [9, 15, 16]. To solve these problems, one should modify the above models.

The Solid-On-Solid model (SOS) is more suitable to describe a real surface's properties than those models described above [8, 17, 18, 19]. This growth model does not exhibit strong corrections to scaling and consequently allows us to determine accurate values of scaling exponents [7, 17, 18]. The Restricted-Solid-On-Solid (RSOS) model(a modified version of the SOS model), proposed by Kim et al. [17], is most important due to its wide applicability, such as for surface roughening modeling via exothermic catalytic reactions on the substrate [8]. Various aspects of the Solid-On-Solid model for surface growth have been studied: the effect of long-range elastic interactions [20], growth processes with correlated noise [21], phase transitions as a function of temperature-like parameters [22], the (001)-surface morphology of GaAs annealed at fixed temperature and pressure, the well explained by annealed version of the RSOS model [23, 24]. Crossover from random to correlated regime [25, 26], relaxation to steady states [27], distribution of local configurations for finite values of S [8], Markov analysis [28], the effect of hopping in various local growth rules on the linear and nonlinear fourth-order dynamical growth equation [29], growth model in higher dimensions [30] and, more recently, the growth on fractal substrates based on the SOS model [31], has also been addressed in the literature.

As mentioned in many previous studies, it is believed that the RSOS model belongs to the Kardar-Parisi-Zhang (KPZ) universality class in the continuum limit [32, 33]. The KPZ equation is one of the most important phenomenological theories in which time evolution of the interface has been characterized by the height function $h(\vec{r}, t)$ at position

 \vec{r} and time t. The governing equation is given by [34]:

$$\frac{\partial h(\vec{r},t)}{\partial t} = \nu \nabla^2 h(\vec{r},t) + \frac{\lambda}{2} [\nabla h(\vec{r},t)]^2 + K(\vec{r},t). \tag{1}$$

Here ν and λ represent the surface tension and the excess velocity respectively, while $K(\vec{r},t)$ is a Gaussian noise with zero mean and co-variance

$$\langle K(\vec{r},t)K(\vec{r'},t')\rangle = D\delta^d(\vec{r}-\vec{r'})\delta(t-t'),$$

where d is the dimension of the substrate, and D is the noise intensity [7, 12]. The interface width reads as:

$$W(L^d, t) = \left\langle \left[\frac{1}{L^d} \sum_{\vec{r}} [h(\vec{r}, t) - \overline{h}(t)]^2 \right]^{1/2} \right\rangle. \tag{2}$$

This characterizes the roughness of the interface, for growth in a substrate of length L, and $\overline{h}(t)$ is the spatial average of height at time t. For short times, the interface scales as follows:

$$W(L,t) \approx t^{\beta} \tag{3}$$

where β is called the growth exponent. For long times, a steady state is attained and the width is saturated as follows:

$$W_{sat}(L,t) \approx L^{\alpha}.$$
 (4)

Here α is the roughness exponent. Equations (3) and (4) correspond to limits of the dynamical relation of the Family and Vicsek ansatz:

$$W(L,t) \approx L^{\alpha} f\left(\frac{t}{L^z}\right).$$
 (5)

The dynamical exponent, $z = \frac{\alpha}{\beta}$, characterizes the crossover from the growth regime to the steady state. The exact scaling exponents are known in d = 1, but no exact value has been obtained in two or more dimensions [16]. Many discrete models fall into the KPZ class, such as the RSOS model [17, 18] and Ballistic Deposition BD [12]. Most of the reported values of α range from $\alpha = 0.37$ to $\alpha = 0.40$ [17, 18, 35, 36, 37], confirmed by numerical solutions of the KPZ equation [38, 39, 40].

The competition between different growth mechanisms during particle deposition, as well as phase transitions which are very often observed in many real growth processes, has been investigated in many studies [25, 26]. Recently, it has been confirmed that there exists a crossover between the Random Deposition and KPZ classes at the initial growth stages for all values of the height restriction parameter between nearest neighbours for the SOS model in 1 + 1-dimension [8]. Here we are interested in investigating the possibility of the existence of crossover in the SOS model in 2 + 1 dimensions. In addition, we give a new approach to determine the roughness exponent using Markovian properties of surfaces.

The rest of this paper is organized as follows: in section 2, we introduce the Markovian surface, and by using the characteristic function, the roughness exponent is calculated. The SOS model for finite values of S is numerically investigated in section 3. Crossover in the growth mechanism and corresponding properties are also investigated

in detail in section 3. Section 4 is devoted to conclusions and summary of our studies.

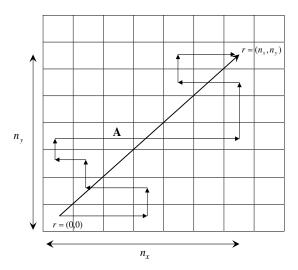


Fig.1 A typical trajectory from point r = (0,0) to $r = (n_x, n_y)$.

2. Markovian Surface

The Markovian surface is one of several models to represent multi-level (stepped) crystalline surfaces. In this model, it is assumed that the steps have only a mono-atomic height. Displacement through any steps may be upward or downward, each occurring with equal probability. Let γ be the probability of meeting an atom displaced vertically either upward or downward in going from any lattice site to an adjacent one. That is, the probability of encountering a step $(\Delta h = \pm 1)$ while the corresponding probability for a lateral walk, namely $\Delta h = 0$ (h is the height of the surface), is equal to $1 - \gamma$. Since every displacement or step occurs independent of any other, the step surface is mapped to the path of a Markovian chain [41]. For the Markovian chain or random walk model, there exist three choices for the displacement at each walk: an upward walk with a probability $\gamma/2$, a downward walk with a probability $\gamma/2$ and a lateral walk with a probability $1-\gamma$ [41]. As mentioned in the introduction, here we rely on the Markovian surface to explore the scaling exponent of the RSOS growth model. To this end, we introduce the characteristic function defined as the Fourier transform of the probability distribution function, $P(\Delta h(\vec{r}))$, with respect to $\Delta h(\vec{r}) = h(\vec{r}) - h(0)$ after saturation time, as

$$Z_d(\lambda, \vec{r}) = \langle e^{i\lambda c[h(\vec{r}) - h(0)]} \rangle \tag{6}$$

where c is the unit of step variations, which is equal to one in the Markovian surface and RSOS model. The height difference, $h(\vec{r}) - h(0)$ can be represented as the sum of the height differences between successive sites from r = 0 to r = na in one-dimension and to $r = \sqrt{(n_x^2 + n_y^2)a}$ in two-dimensions (a is lattice unit). In one-dimension we

have [41]:

$$h(na) - h(0) = \sum_{i=1}^{n} [h(ia) - h((i-1)a)]$$
(7)

For the RSOS model in 2+1 dimensions, the height difference between any sites with coordinates (n_x, n_y) and its nearest neighbour sites with coordinates $(n_x \pm 1, n_y)$ and $(n_x, n_y \pm 1)$ is ± 1 . To calculate the characteristic function, we should move from point $\vec{r} = (0,0)$ to $\vec{r} = (n_x, n_y)$ in different paths like path A as shown in Figure (1). So the vector sum of the trajectories within path A gives the vector \vec{r} . Due to isotropy and homogeneity of the surface, the probability γ is similar for each step. Consequently, the $Z_d(\lambda, \vec{r})$ can be written as follows:

$$Z_{d}(\lambda, \vec{r})|_{A} = \langle e^{i\lambda c[h(\vec{r}) - h(0)]} \rangle|_{A}$$

$$= \langle e^{i\lambda c[h(n_{x}, n_{y}) - h(n_{x} - 1, n_{y})]} \rangle$$

$$\times \langle e^{i\lambda c[h(n_{x} - 1, n_{y} - 1) - h(n_{x} - 2, n_{y})]} \rangle$$

$$\times \langle e^{i\lambda c[h(n_{x} - 2, n_{y}) - h(n_{x} - 2, n_{y} - 1)]} \rangle \cdots$$
(8)

The number of different paths from point r = (0,0) to $r = (n_x, n_y)$ is $(n_x + n_y - 2)$ with the condition $n_x, n_y > 1$ and the number of paths from point r = (0,0) to $r = (n_x, n_y)$ is $N \equiv \mathbf{C}_{n_x + n_y - 1}^{n_x n_y} = (n_x n_y)!/(n_x n_y - n_x - n_y + 1)!(n_x + n_y - 1)!$. Finally the characteristic function $Z_d(\lambda, \vec{r})$ can be written as

$$Z_d(\lambda, \vec{r}) = N f^{n_x + n_y - 2}. \tag{9}$$

Here

$$f \equiv \langle e^{i\lambda c[h(n_x, n_y) - h(n_x - 1, n_y)]} \rangle$$

$$= \int d\Delta h \quad e^{i\lambda c\Delta h(\vec{r})} P(\Delta h(\vec{r}))$$

$$= 1 - \gamma [1 - \cos(\lambda c)]$$
(10)

Therefore, the characteristic function for the RSOS model is

$$Z_d(\lambda, \vec{r}) = N \left\{ 1 - \gamma [1 - \cos(\lambda c)] \right\}^{(n_x + n_y - 2)}$$
(11)

For $r \to 0$ regime and small γ , equation (11) becomes:

$$Z_d(\lambda, \vec{r}) = e^{\gamma[1 - \cos(\lambda c)](n_x + n_y - 2)}$$
(12)

On the other hand, the above equation can be expressed [16] as

$$Z_d(\lambda, \vec{r}) = e^{-\frac{1}{2}\lambda c^2 r^{2\alpha}} \tag{13}$$

By comparing equations (12) and (13), one finds:

$$r^{2\alpha} = \left(n_x^2 + n_y^2\right)^{\alpha}$$

$$\sim (n_x + n_y - 2) \tag{14}$$

In order to determine the roughness exponent, α , we have to compute the following scaling relation for small \vec{r} :

$$n_x + n_y - 2 \sim (n_x^2 + n_y^2)^{\alpha} \tag{15}$$

By using numerical calculations and averaging over small values of \vec{r} , the roughness exponent can be read as 0.39 ± 0.03 in 1σ confidence level, which is in good agreement with the previous results [17, 18, 35, 36, 37].

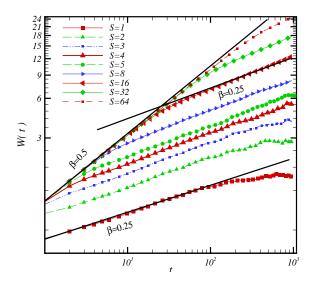


Fig.2 Log-log plot of interface width versus time for various values of parameter S. Here the system size is $L \times L = 4096$, and ensemble averaging has been done over 500 independent runs. Solid lines show the scaling behavior of RD and KPZ models in 2 + 1 dimensions with slopes $\beta = 0.5$ and $\beta = 0.25$, respectively.

3. Simulation of Solid on Solid growth model in 2+1 dimensions

In the previous section, we dealt with the Markovian surface and calculated roughness exponent for restricted solid-on-solid model in a new way. In this section we simulate this surface growth model in 2+1 dimensions for finite values of parameter S on the square lattice with length L. The growth process of the SOS model can be described by the following steps:

Step 1: Select a site randomly e.g. site $\vec{r}:(n_x,n_y)$ among all L^2 sites.

Step 2: Then all of the following conditions should be satisfied to increase the height of mentioned site:

- I) $|[h(n_x, n_y; t) + 1] [h(n_x 1, n_y; t)]| \le S$
- II) $|[h(n_x, n_y; t) + 1] [h(n_x + 1, n_y; t)]| \le S$
- III) $|[h(n_x, n_y; t) + 1] [h(n_x, n_y 1; t)]| \le S$
- IV) $|[h(n_x, n_y; t) + 1] [h(n_x, n_y + 1; t)]| \le S$
- V) Otherwise, do nothing.

Step 3: Repeat the above tasks.

To reduce the errors due to the substrate's boundaries, we use periodic boundary conditions during particle deposition. Each time step is defined as the number of particles needed to fill the surface average, which is equal to $L \times L$ [17, 18]. The log-log plots of the $W(L^2, t)$ versus time scale for SOS model with different values of S are shown in Figure (2). The slope of these diagrams, for the initial time scale of the

growth process, gives the growth exponent, β , of the model. Figure (2) demonstrates that there exists crossover for $t \ll t_{sat}$ in the log-log plot of interface width versus growth time. To investigate the crossover behavior of interface width at small time for various values of parameter S, we define a fluctuation function as:

$$\Delta_{\diamond}(S) = \sum_{t}^{\tau_{\times}(S)} |W(S, t) - W_{\text{The}}^{\diamond}(S, t)| \tag{16}$$

where $W_{\text{The}}^{\diamond}(S,t) \sim t^{\beta_{\diamond}}$ and the symbol \diamond stands for RD and KPZ and corresponding exponents are 0.50 and 0.25, respectively. It is worth noting that RD and KPZ are the most relevant universality classes for SOS growth model reported in [8, 17, 18]. As Figure (3) shows, by increasing the value of the restricted parameter S, deviation(δS) from KPZ(RD) class at the initial growth stage increases(decreases). After enough time, the interface width of SOS model in 2+1 dimensions will be saturated. The value of S for the intermediate value of fluctuation function (equation (16)) is $S_{\times} = S$. Subsequently one concludes the SOS model in 2+1 dimensions for approximately $S \geq S_{\times}$ and before saturation epoch belongs to the two different universal classes: at the very early growth stage, it belongs to the RD class and at intermediate time scales, $t_{\times} < t \ll t_{sat}$, it tends to the KPZ universality class and is affected by the restrictions on the height differences or behaves like the RSOS model with S = 1. On the other hand, for $S < S_{\times}$, the SOS model only belongs to one class, namely, KPZ class, before the saturation of its interface width. The mathematical form of this dynamic for $S \geq S_{\times}$ can be read as

$$W(S,t) = W(S)f\left(\frac{t}{\tau_{\times}}\right) \tag{17}$$

in which

$$f\left(\frac{t}{\tau_{\times}}\right) \sim \begin{cases} \left(\frac{t}{\tau_{\times}}\right)^{0.50} & t < \tau_{\times} \\ \left(\frac{t}{\tau_{\times}}\right)^{0.25} & \tau_{\times} < t \ll L^{z} \end{cases}$$
 (18)

where τ_{\times} is the crossover time scale indicating transition from random deposition universality class to RSOS class which in principle depends on S. The quantity W(S) just depends on S. Recently Ching-Chun Chien et al.[8] have shown that the growth exponent, β , for SOS model in 1+1 dimensions during the very early stage of surface growth is independent of S. Their results confirmed that SOS model in 1+1 dimensions for $t < t_{\times}$ belongs to RD class and then crosses over to the KPZ universality class for $t_{\times} < t \ll t_{sat}$, while the extension of their results to 2+1 dimensions demonstrates that for $S < S_{\times}$, it belongs to only one universality class for $t \ll t_{sat}$ (Figure (3)).

In order to interpret the crossover in the interface width function (see Figure (2)), we refer to the correlation function, $C(\vec{r}, \vec{r'})$ defined by

$$C(\vec{r}, \vec{r'}) = \langle [h(\vec{r}, t) - \bar{h}][h(\vec{r'}, t) - \bar{h}] \rangle \tag{19}$$

For an isotropic surface, we can define the normalized correlation function as follows:

$$C(|\vec{r} - \vec{r'}|) = \frac{\langle [h(\vec{r} + \vec{l}, t) - \bar{h}][h(\vec{r}, t) - \bar{h}]\rangle}{\langle [h(\vec{r}, t) - \bar{h}]^2 \rangle}$$
(20)

The correlation functions for various values of S at the early time scale, $t \ll t_{sat}$, are shown in Figure (4). The correlation length scale, over which the correlation function reaches 1/e of its maximum, decreases as S increases. Moreover, as S increases the effect of randomness in the particle deposition process decreases. This can be explained as follows: for larger values of S, during the very early stage of surface growth, the height of a typical site is not affected by its neighbouring sites due to the restriction constraint embedded in the rule of its deposition. Consequently, one expects the correlation length of height to decrease as S increases at the very early stage of growth. Therefore, the SOS model with infinite S reduces to the RD model during the very early growth stage. Figure (5) indicates the log-log plot of time in which the SOS model crosses over from RD class to KPZ class, τ_{\times} versus S. This confirms the scaling behaviour of transition time versus height difference. The slope of this plot is $\eta = 1.99 \pm 0.02$ at 1σ confidence interval. This value is in agreement with results in 1+1 dimensions given by Chih-Chun Chien et al. [8]. It may be stated that exponent has the same values in 1 and 2-space dimensions, while the growth and roughness (see below) exponents depend on space dimension.

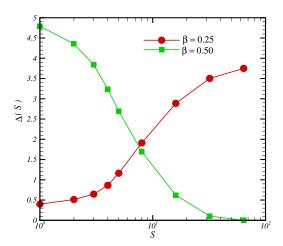


Fig.3 The function of $\Delta(S)$ for $\beta_{\text{KPZ}} = 0.25$ (filled circle symbol) and $\beta_{\text{RD}} = 0.50$ (filled square symbol) at $t \ll t_{sat}$.

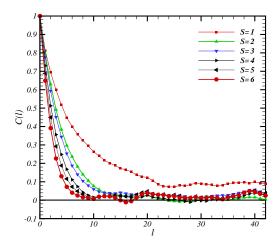


Fig.4 Correlation functions for SOS model for different values of height restriction parameters.

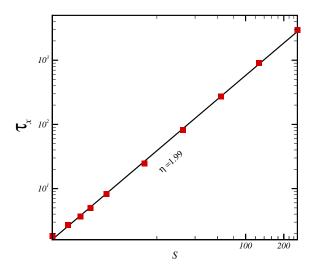


Fig.5 The crossover time scale as a function of parameter S. Solid line indicates the scaling function with exponent, $\eta = 1.99$.

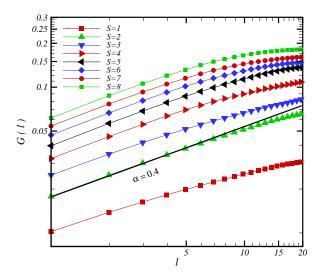


Fig.6 Log-log plot of height correlation function versus separation distance for various values of S. Solid line corresponds to scaling function with exponent, $\alpha = 0.40$.

Another interesting parameter is the roughness exponent, α , which is also given via the structure function for each S as follows: let the structure function be defined as

$$G(\vec{r}, \vec{r'}; t) = \langle [h(\vec{r}, t) - h(\vec{r'}, t)]^2 \rangle^{1/2}.$$
 (21)

In the homogeneous and isotropic case G depends on time scale, t and separation distance, $l = |\vec{r} - \vec{r'}|$. In addition, in principle this function may depend on S, so in the most general case, the structure function reads as:

$$G(l, S; t) = G(l, S)g\left(\frac{t}{l^z}\right)$$
(22)

where $z = \alpha/\beta$. The roughness saturates after a sufficiently long time; consequently $G(l, t > t_{sat})$ behaves as:

$$G(l, S_{\text{fixed}}, t > t_{sat}) \equiv G(l, S_{\text{fixed}}) \approx l^{\alpha}$$
 (23)

Therefore, the slope of log-log plot of $G(l, S_{\text{fixed}})$ versus l for small separation distance in the saturation regime gives the roughness exponent, α . Figure (6) shows the structure function for different values of S in the saturation regime. The slopes of $G(l, S_{\text{fixed}})$ for small l are all equal to 0.40 ± 0.01 at 1σ confidence level which is the same as that determined for the KPZ model in 2+1 dimensions. This confirms that the SOS model belongs to the KPZ universality class during the late growth stage. Figure (7) shows the log-log plot of G(l, S) for small separation distance and fixed l versus S. It demonstrates a scaling behavior for structure function in the saturation regime for small and fixed l as a function of S. Its scaling exponent is equal to $\xi = 0.86 \pm 0.05$, at 68% confidence level. We introduce a new scaling function which gives the relation between l and S after saturation epoch:

$$G(l,S) = l^{\alpha} u\left(\frac{S}{l^{z'}}\right) \tag{24}$$

Dimension	β	η	α	ξ
1+1	All S [8] $t < t_{\times} 0.5$ $t > t_{\times} 0.33$	2.06 [8]	0.5	0.92 ± 0.05
2+1	$S < S_{\times} 0.25$ $S > S_{\times} t < t_{\times} 0.5$ $S > S_{\times} t > t_{\times} 0.25$	1.99 ± 0.02	0.40 ± 0.01	0.86 ± 0.05

Table 1. Values of the scaling exponents of SOS growth model in 1 + 1 and 2 + 1 dimensions.

where $z' = \frac{\alpha}{\xi}$ which is a new dynamical exponent. We also examined the height-height correlation function in 1+1 dimensions for various values of S. Our results confirm a scaling behavior with the exponent equal to $\xi = 0.92 \pm 0.05$. Table (1) reports all the most relevant exponents determined in this paper as well as those given in ref. [8].

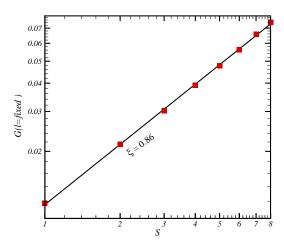


Fig.7 Log-log plot of G(l = fixed) versus S in 2+1 dimensions. Solid line shows the scaling function with slope $\xi = 0.86$.

4. Summary and conclusion

In this paper, we explored some scaling properties of the Solid On Solid model, one of the well-established algorithms for surface growth in 2+1 dimensions. The scaling properties of the model give deep insight into its universality and statistical classification. To this end, we have proposed a new method for finding the roughness exponent for one of the special classes of the SOS model: the so-called RSOS model. In the RSOS model, the value of near-neighbours height difference is restricted to S=1. This new method uses Markovian surfaces properties. By introducing a characteristic function

we computed the scaling behavior of the site's numbers with respect to the various values of the displacement vector. The value of the roughness exponent derived by the Markovian approach is $\alpha = 0.39 \pm 0.03$ at 68.3% confidence interval. Our result for the roughness exponent is in good agreement with those obtained from direct simulation of the RSOS model performed in earlier works [17, 18, 35, 36, 37]. We simulated the growth surface according to the SOS algorithm explained in section 3 for finite values of S. The interface width as a function of time has a crossover time scale for approximately $S \geq 8$ which confirms two universality classes for the SOS model at the very early stage of its growth. The SOS model for $S \geq 8$ at $t < \tau_{\times}$ falls under the random deposition universality class and thereafter tends to the KPZ universality class for $t_{\times} < t \ll t_{sat}$. To make these crosses over more obvious, we investigated the normalized correlation function. Our results indicate that by increasing the height difference parameter at $t \ll t_{sat}$, the correlation length scale is decreased (see Figure (4)). This is clearly due to the restriction constraints which eliminate the effect of neighbors on the memory of particle deposition. With increasing growth time, particle depositions are affected by the restriction rule; consequently, the SOS model with infinite S tends to the KPZ growth model before the saturation time stage. According to Figure (5), the scaling exponent of τ_{\times} versus S is $\eta = 1.99 \pm 0.02$ which is in agreement with that obtained in 1+1 dimensions [8], while the growth and roughness exponents depend on the space dimension. In order to compute the roughness exponent, we used a structure function. The slope of this structure function versus distance separation, l in the log-log scale for various values of parameter S is $\alpha = 0.40 \pm 0.01$ at 68% confidence level. This quantity, in contrast to the growth exponent, did not show crossover behaviour in the log-log plot of structure function as a function of separation distance (see Figure (6)). The value of the roughness exponent also confirms our result regarding the universality class of the SOS model at longer times. Based on Figure (7), we found that the height-height correlation function, G(l) for small and fixed l versus S indicates a scaling behavior with exponent ξ which is equal to 0.86 ± 0.05 and $\xi = 0.92 \pm 0.05$ at 1σ level of confidence for 2+1 and 1+1 dimensions, respectively. Using the roughness and ξ exponents we introduced a new dynamical exponent as $z' = \alpha/\xi$.

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